

Confining electrons on a topological insulator surface using potentials and a magnetic field

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We study the effects of extended and localized potentials and a magnetic field on the Dirac electrons residing at the surface of a three-dimensional topological insulator. We use a lattice model to numerically study the various states; we show how the potentials can be chosen in a way which effectively avoids the problem of fermion doubling on a lattice. We show that extended potentials of different shapes can give rise to states which propagate freely along the potential but decay exponentially away from it. For an infinitely long potential barrier, the dispersion and spin structure of these states are unusual and these can be varied continuously by changing the barrier strength. In the presence of a magnetic field applied perpendicular to the surface, these states become separated from the gapless surface states by a gap, thereby giving rise to a quasi-one-dimensional system. Similarly, a magnetic field along with a localized potential can give rise to exponentially localized states which are separated from the surface states by a gap and thereby form a zero-dimensional system. Finally, we show that a long barrier and an impurity potential can produce bound states which are localized at the impurity, and an “L”-shaped potential can have both bound states at the corner of the “L” and extended states which travel along the arms of the potential.

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I. INTRODUCTION

Topological insulators (TIs) are materials which have gapped states in the bulk and gapless states on the boundaries which are protected by time-reversal symmetry^{10,11}. These materials have been studied both theoretically¹⁻⁵ and experimentally⁶⁻⁹ for a number of years. Three-dimensional TIs such as Bi₂Se₃, Bi₂Te₃ and Sb₂Te₃ have surfaces on which there is a single species of gapless states which is governed by the Dirac equation⁷⁻⁹. A number of interesting properties of the surface states of a TI have been studied⁹⁻²¹. Junctions of different surfaces of TIs, sometimes separated by a geometrical step or a magnetic domain wall²⁴⁻³², junctions of surfaces of a TI with normal metals or magnetic materials⁴⁴ or superconductors⁴⁵, and polyhedral surfaces³³ have been investigated. The effects of finite sizes³⁴⁻³⁹ and different orientations^{30,40-43}, and transport around different surfaces of a TI in the presence of a magnetic field⁴⁶ have been studied. The effect of a periodically varying one-dimensional potential and a magnetic field on the spectrum of electrons on the surface of Bi₂Te₃ has been studied in Ref. 47.

It is known analytically that an infinitely long δ -function potential barrier running along the x axis applied to the $x - y$ surface of a TI gives rise to states which propagate as plane waves along the barrier and decay exponentially away from it²⁵. However, there is no energy gap between the states produced by the potential barrier and the gapless surface states which exist far from the potential. As a result, the former states are not robust against disorder; even a weak disorder can produce a transition between these states and the gapless surface states. On the other hand, a potential localized in some region does not produce any localized

states. If we now apply a Zeeman field perpendicular to the surface, the surface states get gapped out. It is then possible that localized potentials will also produce localized states, and that the states produced by various potentials (either extended or localized) will lie in the gap of the surface states and will therefore be stable against weak disorder. Hence, we can produce systems confined to one or zero dimensions (resembling quantum wires and dots) which may be useful for various practical applications.

In this paper, we use a lattice model to study the states produced by a combination of non-magnetic potentials and a perpendicular magnetic field which is Zeeman coupled to the spin of the electrons. A lattice model allows us to numerically study the effects of potentials of any magnitude and shape. The plan of our paper is as follows. In Sec. II, we review the Dirac Hamiltonian in the continuum and its symmetries in the presence of a potential and a magnetic field. In Sec. III we discretize the Hamiltonian using a square lattice and we discuss the fermion doubling problem that arises for Dirac electrons. In Sec. IV, we numerically study the spectrum of electrons in the presence of an infinitely long potential barrier which is taken to have a Gaussian profile in the transverse direction. Since this system has translation invariance along one direction, the momentum along that direction is a good quantum number and can be used to reduce it to a one-dimensional problem. In the absence of a magnetic field, the dispersion of the states propagating along the barrier (henceforth called edge states) is qualitatively found to be of the form $E = v|k_x|$, where k_x is the momentum along the barrier, if $|k_x|$ is much smaller than the inverse lattice spacing. The expectation value of the spin, $\langle \vec{\sigma} \rangle$, of the edge states lies in the y direction. The velocity v of the the edge states is smaller than that

of the surface states and it can be varied by changing the strength of the potential barrier. The velocity v is found to be very small for a particular value of the potential barrier, giving rise to an almost flat band near $E = 0$. The wave function of the edge states decays exponentially away from the potential barrier; the decay length is found to be inversely proportional to $|k_x|$. Hence the edge states will cease to exist when the decay length becomes comparable to the size of the system. When a Zeeman field is applied in the z direction, the surface states become gapped but the edge states do not. Further, the edge state now exists even for $k_x = 0$, and their dispersion can be controlled by the potential barrier. The edge states then define a tunable one-dimensional system which is separated from the surface states by a gap. In Sec. V, we study the effects of a variety of potentials with two-dimensional profiles. We first consider a potential localized in some region. In the absence of a Zeeman field there are no localized states, but when a Zeeman field is turned on, we find that there exponentially localized states can appear if the potential is strong enough. Next, we study a combination of a long potential barrier, a localized potential and a magnetic field; we find that states can appear which are bound to the localized potential. Finally, we study what happens if there is an “L”-shaped potential consisting of two infinitely long arms meeting at a corner and a magnetic field. We find that there can be both states bound to the corner of the “L” as well as scattering states which propagate along the arms. In Sec. VI, we summarize our main results and describe some ways of experimentally testing these results.

II. SURFACE HAMILTONIAN

The surface states of a three-dimensional TI are governed by the massless Dirac equation. The form of the Dirac equation depends on the orientation of the surface^{30,40–43}; the simplest form appears when the surface is given by the $x - y$ plane. We will also be interested in the effects of a scalar potential $V(x, y)$ and a uniform magnetic field \vec{B} which only has a Zeeman coupling to the electrons. Including these terms, the two-component wave function $\psi(x, y)e^{-iEt}$ of an energy eigenstate satisfies the equation

$$[-iv_F(\sigma^x \partial_y - \sigma^y \partial_x) + V - \frac{g\mu}{2} \vec{\sigma} \cdot \vec{B}] \psi = E\psi, \quad (1)$$

where v_F , μ and g denote the Fermi velocity, the Bohr magneton, and the gyromagnetic ratio respectively. (We will set $\hbar = 1$ in this paper).

Spin-momentum locking: If both V and \vec{B} are absent, the solutions of Eq. (1) have momenta $\vec{k} = (k_x, k_y)$ and energies $E_{\pm} = \pm v_F \sqrt{k_x^2 + k_y^2}$. The wave functions

are given by $\psi e^{i(k_x x + k_y y - Et)}$, where

$$\begin{aligned} \psi_+ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{k_y - ik_x}{E} \end{pmatrix} \text{ for } E_+, \\ \psi_- &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\frac{k_y - ik_x}{E} \end{pmatrix} \text{ for } E_-. \end{aligned} \quad (2)$$

Upon calculating the expectation values $\langle \sigma^x \rangle$, $\langle \sigma^y \rangle$ and $\langle \sigma^z \rangle$, we find that the direction of spin is perpendicular to both \hat{z} and $\hat{k} = \vec{k}/|\vec{k}|$, namely, $\langle \vec{\sigma} \rangle = \hat{k} \times \hat{z}$ and $-\hat{k} \times \hat{z}$ for E_+ and E_- respectively. This property of the surface states is called spin-momentum locking.

If we now turn on a magnetic field perpendicular to the surface, $\vec{B} = B_z \hat{z}$, the states with momentum (k_x, k_y) will have energies $E_{\pm} = \pm \sqrt{v_F^2(k_x^2 + k_y^2) + (g\mu B_z/2)^2}$; hence there will be a gap of $|g\mu B_z|$ at $\vec{k} = 0$. Further, these states have a non-zero value of $\langle \sigma^z \rangle$.

Effect of a potential: Let us now turn on a potential $V(x, y)$ but no magnetic field \vec{B} . Then Eq. (1) takes the form

$$[v_F(-i\sigma^x \partial_y + i\sigma^y \partial_x) + V(x, y)] \psi = E\psi. \quad (3)$$

Eq. (3) has the following symmetries.

(i) Time-reversal symmetry \mathcal{T} : Eq. (3) remains invariant if we complex conjugate all numbers, and transform and $\psi(x, y) \rightarrow \sigma^y \psi^*(x, y)$. Since $\sigma^{y*} = -\sigma^y$, we have $\mathcal{T}^2 = -I$; this implies that every energy level must have a two-fold degeneracy.

(ii) Parity symmetry \mathcal{P} : If the potential is invariant under reflection in y , i.e., $V(x, -y) = V(x, y)$, we have a symmetry \mathcal{P} under which $\psi(x, y) \rightarrow \psi^*(x, -y)$.

(iii) π -rotation symmetry \mathcal{R} : If the potential is invariant under a π rotation about the \hat{z} axis, i.e., $V(-x, -y) = V(x, y)$, we have a symmetry \mathcal{R} under which $\psi(x, y) \rightarrow \sigma^z \psi(-x, -y)$.

If a magnetic field is applied in the z direction, time-reversal symmetry is broken but \mathcal{P} and \mathcal{R} hold if V has both parity and rotational symmetries.

In Ref. 25, the effect of a δ -function potential barrier, $V(y) = V_0 \delta(y)$, was studied analytically. It was shown that this can give rise to states which propagate as plane waves in the x direction and decay exponentially as one moves away from $y = 0$. In the next section, we will consider the effect of more complicated potentials as well as a magnetic field applied in the z direction.

III. LATTICE MODEL AND FERMION DOUBLING

For a general form of the potential $V(x, y)$, for example in the presence of impurities, it is not possible to find the energy spectrum and wave functions analytically and one has to resort to a numerical solution. For this purpose, we assume the $x - y$ plane to be a lattice of discrete points

$\{n_x, n_y\}$ and Eq. (1) becomes,

$$-\frac{1}{2}(\beta_{n_x+1, n_y} - \beta_{n_x-1, n_y}) - \frac{i}{2}(\beta_{n_x, n_y+1} - \beta_{n_x, n_y-1}) + (V_{n_x, n_y} + B)\alpha_{n_x, n_y} = E\alpha_{n_x, n_y}, \quad (4)$$

$$\frac{1}{2}(\alpha_{n_x+1, n_y} - \alpha_{n_x-1, n_y}) - \frac{i}{2}(\alpha_{n_x, n_y+1} - \alpha_{n_x, n_y-1}) + (V_{n_x, n_y} - B)\beta_{n_x, n_y} = E\beta_{n_x, n_y}, \quad (5)$$

where α_{n_x, n_y} and β_{n_x, n_y} respectively denote the wave functions of spin- \uparrow and spin- \downarrow electrons at the site $\{n_x, n_y\}$, we have assumed a magnetic field $\vec{B} = B_z \hat{z}$ with $B = -g\mu B_z/2$. In our numerical calculations, we will work in units in which the velocity v_F and lattice spacing a are both equal to unity; at the end of Sec. V we will restore all the physical units for a topological insulator like Bi_2Se_3 .

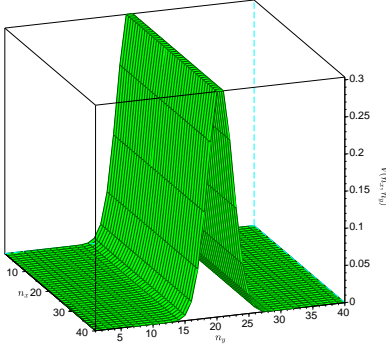


FIG. 1: Surface plot of a potential barrier which is a Gaussian in one direction with width 2 and $V_b = \pi/2$, as described in Eq. (14).

Fermion doubling: Eqs. (4-5) suffer from the problem of “fermion doubling”. To see this in the simplest possible way, consider the case when both the potential and the magnetic field are absent, i.e., $V = 0$ and $B = 0$. Translational symmetry along both x and y directions allows the solution

$$\begin{pmatrix} \alpha_{n_x, n_y} \\ \beta_{n_x, n_y} \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} e^{i(k_x n_x + k_y n_y)}. \quad (6)$$

This gives

$$\begin{aligned} [\sin(k_y) - i \sin(k_x)] \beta &= E\alpha, \\ [\sin(k_y) + i \sin(k_x)] \alpha &= E\beta, \end{aligned} \quad (7)$$

which leads to the dispersion relation

$$E = \pm \sqrt{\sin^2(k_x) + \sin^2(k_y)}. \quad (8)$$

Clearly this vanishes at four points in the Brillouin zone lying at $(0, 0)$, $(0, \pi)$, $(\pi, 0)$ and (π, π) , giving rise to four

Dirac cones, in contrast to the continuum theory which only has one Dirac cone at $(0, 0)$.

One way to avoid this problem is to add the Wilson term; this is proportional to σ^z and it adds $w[2 - \cos(k_x) - \cos(k_y)]\alpha_{n_x, n_y}$ in Eq. (4) and $-w[2 - \cos(k_x) - \cos(k_y)]\beta_{n_x, n_y}$ in Eq. (5) on the left hand sides. The dispersion relation now becomes,

$$E = \pm [\sin^2(k_x) + \sin^2(k_y) + w^2(2 - \cos(k_x) - \cos(k_y))^2]^{1/2}. \quad (9)$$

This reduces to Eq. (8) in the low momentum limit, but it does not vanish near the boundaries of the Brillouin zone where k_x or k_y approaches $\pm\pi$. We thus recover a system with only one Dirac cone lying at $(0, 0)$.

Since the Wilson term is proportional to σ^z , it looks like a magnetic field in the z direction; hence it breaks some symmetries such as time-reversal symmetry and gives rise to various spurious effects. We can avoid working with a Wilson term if we can ensure that the wave functions that we are studying only have momentum components lying close to $(k_x, k_y) = (0, 0)$. This will be true if our potentials are sufficiently smooth so that their Fourier components rapidly approach zero as we move away from $(0, 0)$, and if our system sizes are large (since the smallest possible momentum is inversely proportional to the system size). Our numerical results presented below will show that choosing smooth potentials enables us to effectively avoid the fermion doubling problem even without adding a Wilson term.

Bound states and inverse participation ratio: In our numerical studies, we will be specially interested in states which are localized in certain regions of space. We will refer to all such states as bound states for simplicity. Bound states can be identified most easily by inverse participation ratios (IPR) of all the energy eigenstates. Let $\psi_{i; n_x, n_y}$ be the value of the wave function at the lattice site (n_x, n_y) with the i^{th} energy eigenvalue E_i . The normalization condition implies that

$$\sum_{n_x, n_y} |\psi_{i; n_x, n_y}|^2 = 1. \quad (10)$$

We now define

$$(IPR)_i = \sum_{n_x, n_y} |\psi_{i; n_x, n_y}|^4. \quad (11)$$

The more localized the wave function of a particular state is, the higher will its IPR be. This can be understood from following example. If a normalized wave function has the form

$$\psi_{n_x, n_y} \sim \frac{e^{-(n_x^2 + n_y^2)/\xi^2}}{\xi}, \quad (12)$$

its IPR will be proportional to $1/\xi^2$. Hence the state with the smallest width ξ will have the largest IPR.

IV. NUMERICAL RESULTS IN ONE DIMENSION

We first study the energy spectrum in the presence of a potential V which is only a function of n_y on a lattice. The spectrum can be found assuming the wave function to have a momentum k_x along the x direction; this reduces it to a one-dimensional problem involving $\psi = (\alpha_{n_y}, \beta_{n_y})^T e^{i(k_x x - Et)}$. The eigenvalue problem is given by

$$\begin{aligned} -i \sin(k_x) \beta_{n_y} - \frac{i}{2}(\beta_{n_y+1} - \beta_{n_y-1}) + V_{n_y} \alpha_{n_y} \\ = E \alpha_{n_y}, \\ i \sin(k_x) \alpha_{n_y} - \frac{i}{2}(\alpha_{n_y+1} - \alpha_{n_y-1}) + V_{n_y} \beta_{n_y} \\ = E \beta_{n_y}. \end{aligned} \quad (13)$$

We take the potential to be a barrier which is a Gaussian with an integrated weight of

$$V_{n_y} = \frac{V_b}{\sigma\sqrt{2\pi}} e^{-(n_y - n_0)^2/(2\sigma^2)}, \quad (14)$$

with maximum value $V_b/(\sigma\sqrt{2\pi})$ and width σ . In our calculations, we will set the width $\sigma = 2$ and vary V_b . We will take the Gaussian to be centered at $n_y = n_0 = 151$ for a system with 301 sites in the y direction. For $\sigma = 2$, the Fourier transform $\tilde{V}_{k_y} = \sum_{n_y} e^{-ikn_y} V_{n_y}$ decreases rapidly as we go away from $k_y = 0$ and is very small at $k_y = \pi$. Using the Poisson resummation formula, we obtain

$$\left| \frac{\tilde{V}_{k_y}}{\tilde{V}_{k_y=0}} \right| = \frac{\sum_{n=-\infty}^{\infty} e^{-2\pi^2\sigma^2[n-k_y/(2\pi)]^2}}{\sum_{n=-\infty}^{\infty} e^{-2\pi^2\sigma^2 n^2}}, \quad (15)$$

For $\sigma = 2$, we find that Eq. (15) is very well approximated by the Gaussian $e^{-2k_y^2}$ for k_y lying in the range $[-\pi, \pi]$. At $k_y = \pi$, $|\tilde{V}_\pi/\tilde{V}_0| \simeq 3 \times 10^{-9}$ which is extremely small. Hence a Gaussian potential with width 2 is sufficiently smooth so that states near $k_y = \pi$ make very little contribution to the bound states. Indeed, as mentioned below, we find numerically that the wave functions of the energy eigenstates are quite smooth, with period 2 oscillations (corresponding to components of k_y close to π) being rather small.

Bound states: We first consider the case when no magnetic field is applied. As V_b is increased from zero, we find that a set of bound states appears which are separated from the plane wave surface states which have the gapless spectrum $E = \pm\sqrt{k_x^2 + k_y^2}$. The new states are plane waves along the x direction and decay exponentially as one moves away from the centre of the barrier. The energy E of these states is a function of $|k_x|$; this is a consequence of both the symmetries \mathcal{P} and \mathcal{R} mentioned earlier. The ratio $dE/d|k_x|$ close to $k_x = 0$ varies with the potential strength V_b ; it has a value of $-v_F = -1$

close to $V_b = 0$ and increases as V_b is increased, becoming almost zero around $V_b = \pi/2$. This is illustrated in the top panels of Fig. 2, with $V_b = \pi/4$ and $\pi/2$ in Figs. 2 (a) and (b) respectively. $(E/|k_x|)$ becomes positive when V_b is increased beyond $\pi/2$.

We thus see that an almost flat band can be produced by tuning the barrier strength V_b . For such a band, states with different momenta can be superposed suitably to give any wave function that one chooses, and all such states will have almost the same energy. Further, such states will move only slowly in time since the group velocity dE/dk_x is close to zero.

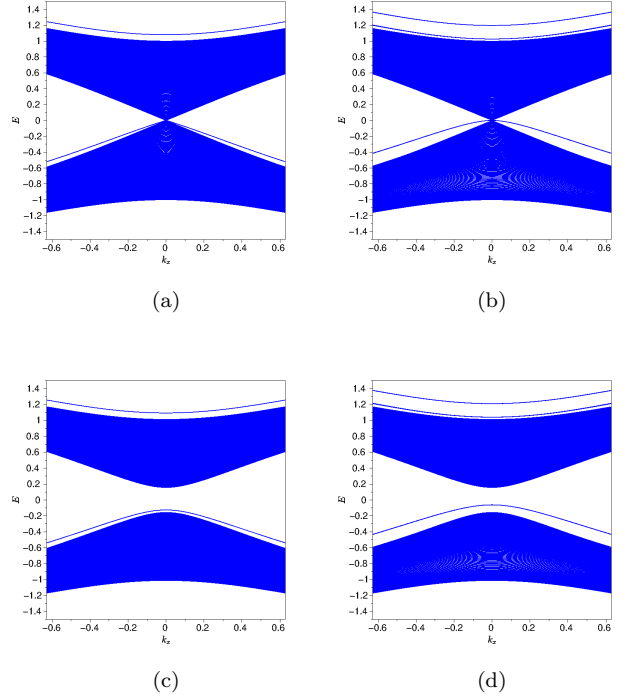


FIG. 2: Energy dispersion of barrier states for (a) $V_b = \pi/4$ and $B = 0$, (b) $V_b = \pi/2$ and $B = 0$, (c) $V_b = \pi/4$ and $B = \pi/20$, and (d) $V_b = \pi/2$ and $B = \pi/20$, for k_x lying in the range $[-\pi/5, \pi/5]$.

The states bound to the potential barrier are degenerate with the surface states. In the presence of scattering (induced by, say, impurities which may be present close to the barrier), an electron occupying a bound states can scatter into a surface state. The bound states can be made immune to such scattering by introducing a magnetic field. Figs. 2 (c) and (d) show the bound states when a magnetic field given by $B = \pi/20$ is introduced. This opens a gap of $2B$ in the spectrum of the surface states, and the bound states which lie within this gap can be expected to be robust against scattering from impurities.

We note that Figs. 2 show some additional sets of states near above the top of the band of surface states. The

wave functions of these states oscillate rapidly on the scale of a lattice spacing (they have momentum components close to π); hence, they are lattice artifacts and have no counterparts in the continuum limit of the model.

The states produced by the potential barrier have probabilities which decay exponentially as we go away from the centre of the Gaussian. The probabilities of spin- \uparrow and \downarrow are given by $|\alpha_{n_y}|^2$ and $|\beta_{n_y}|^2$ respectively. For $B = 0$, these are shown in Figs. 3 (a), (c) and (e) for states with $k_x = -\pi/10$, 0 and $\pi/10$ respectively. We see that for $k_x = 0$, the probability is spread over the entire range of n_y . (The probability looks like a band because it oscillates between 0 and 0.007 with period 2 in n_y). Hence this state is not localized; this will be studied further below using the decay length.

Note that all the bound states shown in Figs. 3, namely, (a), (b), (d), (e) and (f), have probability profiles which are quite smooth; they have small oscillations with period 2 in n_y due to fermion doubling, but these are not visible in the figures. This implies that choosing a smooth potential profile has enabled us to essentially bypass the fermion doubling problem.

For $B = \pi/20$, Figs. 3 (b), (d) and (f) show the probabilities for $k_x = -\pi/10$, 0 and $\pi/10$ respectively. In this case, the $k_x = 0$ state is also localized. In Figs. 3 (b), (d) and (f), the spin- \downarrow probabilities are larger than the spin- \uparrow probabilities because of the presence of a magnetic field $B > 0$. In all the plots in Figs. 3 we observe that the probabilities of spin- \uparrow and \downarrow get reflected about the centre of the Gaussian when we change $k_x \rightarrow -k_x$; this is a consequence of both the symmetries \mathcal{P} and \mathcal{R} .

Decay length: Since the probabilities in Figs. 3 decay rather rapidly (within a few lattice spacings), it is difficult to estimate the decay lengths accurately from these probabilities. The decay length can be estimated more easily from the IPR as follows. Since the states decay in only direction, the probability $|\psi^2|$ will be proportional to $e^{-|n|/\xi}/\xi$ (where n denotes the deviation of n_y from the centre of the Gaussian), and the IPR will be proportional to $1/\xi$. We therefore simply define the decay length ξ to be the inverse of the IPR and plot the resultant values of ξ versus the momentum k_x . We find that ξ is proportional to $1/|k_x|$, the constant of proportionality being almost the same for the probabilities of the spin- \uparrow and \downarrow components. This is shown in Fig. 4 for $V_b = \pi/2$ and $B = 0$. We observe that the decay length diverges as $k_x \rightarrow 0$, implying that there is no bound state at $k_x = 0$. Thus the spectrum of bound states does not contain the point $k_x = 0$. The situation is quite different when a magnetic field is present; then the decay length is finite for all values of k_x and there is a bound state even when $k_x = 0$.

Local density of states: It is useful to look at the local density of states produced by the potential barrier. For the case $V_b = \pi/2$ and $B = \pi/20$ where there is an almost flat band (Fig. 2 (d)), the local density of states produced by the bound states lying in the range $-\pi/5 <$

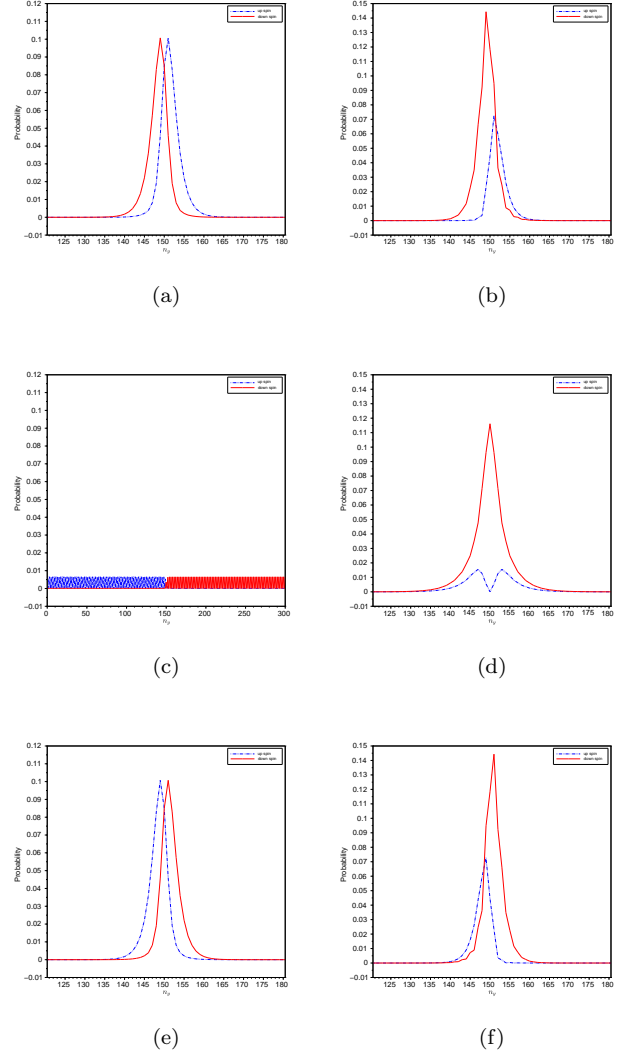


FIG. 3: Probabilities of barrier states for $V_b = \pi/2$ and (a) $B = 0$, $k_x = -\pi/10$, (b) $B = \pi/20$, $k_x = -\pi/10$, (c) $B = 0$, $k_x = 0$, (d) $B = \pi/20$, $k_x = 0$, (e) $B = 0$, $k_x = \pi/10$, (f) $B = \pi/20$, $k_x = \pi/10$. The probabilities of spin- \uparrow and \downarrow are shown in blue (dashed line) and red (solid line) respectively.

$k_x < \pi/5$ is defined to be

$$\rho(E, n_y) = \int_{-\pi/5}^{\pi/5} \frac{dk_x}{2\pi} \delta(E - E_{k_x}) |\psi(k_x; n_y)|^2. \quad (16)$$

This is shown in Fig. 5 where we have smoothened the δ -functions in Eq. (16) by replacing them by Gaussians with width 0.1. (We have approximated the integral in Eq. (16) by taking a large number N of equally spaced points in k_x from $-\pi/5$ to $\pi/5$, adding up the contributions from all those points, and dividing by $5N$). As expected from Fig. 2 (d), the local density of states is peaked at an energy of about -0.2 and at $n_y = 151$ where the barrier is located.

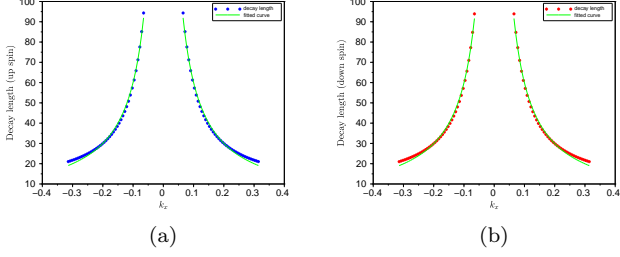


FIG. 4: Estimates of decay length ξ (shown by blue circles) from inverse participation ratio of barrier states for $V_b = \pi/2$ and $B = 0$ for (a) spin- \uparrow and (b) spin- \downarrow . A least square fit of the form $\xi = c/|k_x|$ (shown by green lines) gives $c = 6.00$ for spin- \uparrow and 5.98 for spin- \downarrow .

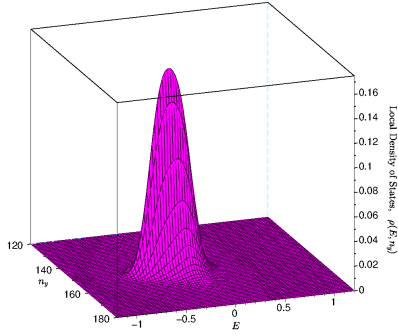


FIG. 5: Local density of states due to bound states produced by a potential barrier with $V_b = \pi/2$ and a magnetic field $B = \pi/20$. The δ -functions in energy have been replaced by Gaussians with width 0.1 .

Spin: It is interesting to look at the expectation values of the different components of the spin as a function of k_x . This is shown in Fig. 6 for $V_b = \pi/2$ and (a) $B = 0$ and (b) $B = \pi/20$. These figures show certain symmetries which can be understood as follows. The symmetry \mathcal{P} under which $\psi(x, y) \rightarrow \psi^*(x, -y)$ implies that $\langle \sigma^y \rangle$ will change sign but $\langle \sigma^x \rangle$ and $\langle \sigma^z \rangle$ will remain the same if we change $k_x \rightarrow -k_x$. The symmetry \mathcal{R} under which $\psi(x, y) \rightarrow \sigma^z \psi(-x, -y)$ implies that $\langle \sigma^x \rangle$ and $\langle \sigma^y \rangle$ will change sign but $\langle \sigma^z \rangle$ will remain the same under $k_x \rightarrow -k_x$. Combining these results, we see that $\langle \sigma^x \rangle$ must be equal to zero for each value of k_x for any value of B ; this agrees with Fig. 6. Finally, if $B = 0$, time-reversal symmetry leads to all three spin expectation values changing sign under $k_x \rightarrow -k_x$. Combined with the symmetries \mathcal{P} or \mathcal{R} , this means that $\langle \sigma^z \rangle$ must equal zero for each value of k_x .

To summarize this section, applying a combination of a translation invariant potential barrier and a magnetic field to Dirac electrons can produce an one-dimensional

system which can be thought of as a one-band quantum wire. The dispersion of this system is unusual in that the energy is an even function of k_x , unlike chiral systems where the energy is an odd function such as $E = vk_x$. The dispersion can be controlled by tuning the barrier strength; in particular, the dispersion can be made almost flat. The wave functions of these states decay exponentially away from the barrier; the decay length increases as $|k_x|$ decreases but remains finite at $k_x = 0$ if a magnetic field is present. The expectation values of the spin components also vary with k_x . We note that all these results are in qualitative agreement with those obtained analytically in Ref. 25 for the case of a δ -function potential barrier.

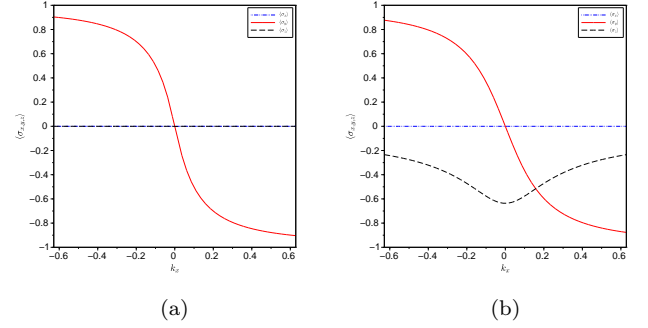


FIG. 6: Spin expectation values of barrier states for (a) $V_b = \pi/2$, $B = 0$, and (b) $V_b = \pi/2$, $B = \pi/20$. The $\langle \sigma^x \rangle$, $\langle \sigma^y \rangle$ and $\langle \sigma^z \rangle$ are shown by blue dot-dash, red solid and black dashed lines respectively. For $B = 0$, $\langle \sigma^x \rangle = \langle \sigma^z \rangle = 0$ coincide.

V. NUMERICAL RESULTS IN TWO DIMENSIONS

In this section, we will present our results for three cases where the potential $V(n_x, n_y)$ does not have translational symmetry along any direction. We will therefore use Eqs. (4-5) to find the spectrum for a two-dimensional system.

Apart from the symmetries \mathcal{T} (if $B = 0$), \mathcal{P} (if $V(n_x, -n_y) = V(n_x, n_y)$) and \mathcal{R} (if $V(-n_x, -n_y) = V(n_x, n_y)$) which the continuum Hamiltonian has, Eqs. (4-5) has two other symmetries which are peculiar to the lattice model. Eqs. (4-5) remain invariant under a transformation \mathcal{A}_x which takes $\psi_{n_x, n_y} \rightarrow (-1)^{n_x} \sigma^z \psi_{n_x, n_y}^*$, and a transformation \mathcal{A}_y which takes $\psi_{n_x, n_y} \rightarrow (-1)^{n_y} \psi_{n_x, n_y}^*$. Combining \mathcal{A}_x and \mathcal{A}_y , we find a symmetry under the transformation \mathcal{A}_{xy} which takes $\psi_{n_x, n_y} \rightarrow (-1)^{n_x + n_y} \sigma^z \psi_{n_x, n_y}$. This implies that the eigenstates of the Hamiltonian can be chosen to satisfy either $\mathcal{A}_{xy}\psi = \psi$ or $\mathcal{A}_{xy}\psi = -\psi$. If $\mathcal{A}_{xy}\psi = \psi$, the spin- \uparrow (spin- \downarrow) component must be zero if $n_x + n_y$ is odd (even), and the situation is reversed if $\mathcal{A}_{xy}\psi = -\psi$. Thus imposing the constraint $\mathcal{A}_{xy}\psi = \psi$ (or $= -\psi$) would

eliminate half the components of ψ_{n_x, n_y} . This is equivalent to the Kogut-Susskind prescription for reducing the fermion doubling problem; the reduction is by a factor of two in this system⁴⁸.

However, we will *not* impose constraints of the form $\mathcal{A}_{xy}\psi = \pm\psi$ when doing our numerical conditions since this would lead to wave functions which have large oscillations of period 2 in n_x and n_y . The various wave functions that we have found numerically and have discussed below are all quite smooth and have only small oscillations of period 2. Once again, this is because we have chosen all the potentials to have very small Fourier components near k_x or k_y equal to π .

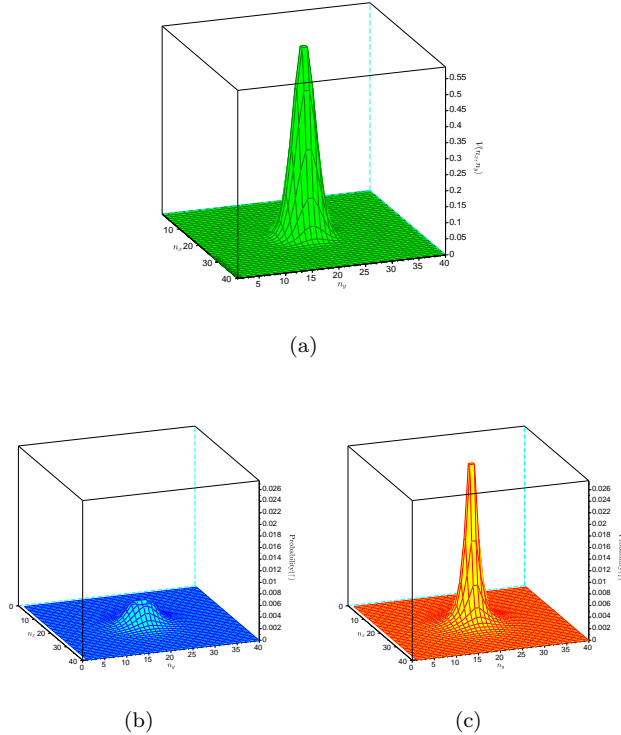


FIG. 7: (a) Surface plot of an impurity potential which is a Gaussian with width 2 in both directions and $V_i = 5\pi$, as described in Eq. (17). Surface plots of probabilities of (b) spin- \uparrow and (c) spin- \downarrow for the bound state, for $B = \pi/20$ and a system with 40×40 sites. The spin- \downarrow probability is much larger than the spin- \uparrow probability; this is because the magnetic field points in the $+\hat{z}$ direction.

Impurity potential: We first consider the effect of a localized potential which may arise from a non-magnetic impurity; by localized we mean that the potential rapidly goes to zero outside some region. In particular, we will consider a Gaussian form

$$V_{imp;n_x, n_y} = \frac{V_i}{2\pi\sigma^2} e^{-[(n_x - n_0)^2 + (n_y - n_0)^2]/(2\sigma^2)}. \quad (17)$$

where $\sigma = 2$ and $V_i = 5\pi$. In the absence of a magnetic field, we find numerically that this potential does not pro-

duce a bound state. However, when we turn on a magnetic field (we take $B = \pi/20$), we find that a localized bound state can appear as shown in Fig. 7. (The inverse participation ratio is particularly large for states which are localized in both directions and is therefore very useful for numerically finding such states). We thus see that while a potential alone does not localize a Dirac electron (since an electron can Klein tunnel through a potential), a potential along with a magnetic field can localize an electron. Qualitatively, this is because a magnetic field produces a gap; if a localized potential can produce a state lying in that gap, the wave function of that state will decay exponentially as one goes far away from the potential thereby producing a localized state. This suggests that one can construct a quantum dot hosting one or more states by applying a localized potential and a magnetic field to a system of Dirac electrons.

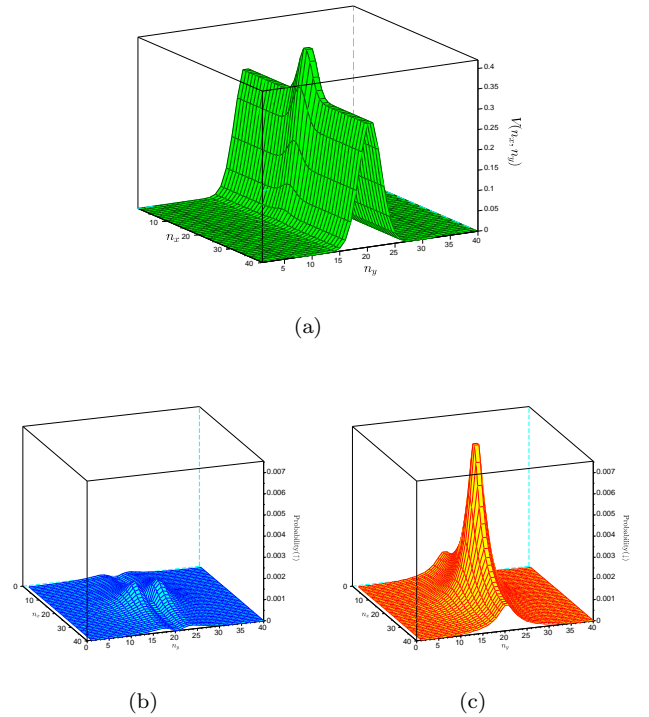


FIG. 8: (a) Surface plot of a potential which is a combination of a barrier which is a Gaussian with width 2 and $V_b = \pi/2$ in the transverse direction and an impurity potential which is a Gaussian with width 2 in both directions and $V_i = \pi$. Surface plots of probabilities of (b) spin- \uparrow and (c) spin- \downarrow for the bound state, for $B = \pi/20$ and a system with 40×40 sites.

Potential barrier and impurity: Next we consider when both a barrier and an impurity are present (both are assumed to be spin independent). In the absence of a magnetic field, the states propagating as plane waves along the barrier are not expected to scatter from the impurity due to time-reversal symmetry. For a weak impu-

rity, this can be shown using first order perturbation theory. For an elastic (i.e., energy conserving scattering), we only need to consider scattering between two plane wave states with equal and opposite momenta $\pm k_x$. Let us denote the corresponding wave functions as $\psi_{k_x; n_x, n_y}$ and $\psi_{-k_x}(n_x, n_y)$. Then the Born approximation in one dimension⁴⁹ shows that the reflection amplitude produced by an impurity $V_{imp; n_x, n_y}$ is given by

$$r_{k_x} = - \frac{i}{dE/dk_x} \langle \psi_{-k_x} | V_{imp} | \psi_{k_x} \rangle. \quad (18)$$

In the absence of a magnetic field, ψ_{\pm} are related by time-reversal transformation:

$$\psi_{-k_x; n_x, n_y} = \sigma^y \psi_{k_x; n_x, n_y}^*. \quad (19)$$

Hence the matrix element in Eq. (18) is equal to

$$\begin{aligned} & \langle \psi_{-k_x} | V_{imp} | \psi_{k_x} \rangle \\ &= \sum_{n_x, n_y} V_{imp; n_x, n_y} \psi_{k_x; n_x, n_y}^T \sigma^y \psi_{k_x; n_x, n_y}. \end{aligned} \quad (20)$$

This vanishes for any form of V_{imp} because the antisymmetry of σ^y implies that $\psi_{k_x; n_x, n_y}^T \sigma^y \psi_{k_x; n_x, n_y} = 0$. Thus the barrier states are immune to scattering by weak impurities if no magnetic field is present. This also implies that an impurity cannot produce a bound state. This is because bound states in one dimension occur at the complex values of k_x where r_{k_x} has a pole (when r_{k_x} is analytically continued away from the real axis); if $r_{k_x} = 0$ for all k_x , its analytical continuation will also be zero and it will have no pole in the complex plane.

These arguments break down when a magnetic field is present because $\psi_{\pm k_x}$ will no longer be related to each other by Eq. (19), and $\langle \psi_{-k_x} | V_{imp} | \psi_{k_x} \rangle$ will not be equal to zero in general; hence the reflection amplitude in Eq. (18) will no longer vanish. In addition, a bound state becomes possible. This is illustrated in Fig. 8 where the spin- \uparrow and \downarrow probabilities are shown for a bound state which appears when there is a potential barrier and an impurity with the forms given in Eqs. (14) and (17) with $V_b = \pi/2$ and $V_i = \pi$ respectively, and a magnetic field $B = \pi/20$ is also present. The spin- \downarrow probability again turns out to be much larger than the spin- \uparrow probability because the magnetic field points in the $+\hat{z}$ direction.

Assuming that a magnetic field is present and $\langle \psi_{-k_x} | V_{imp} | \psi_{k_x} \rangle \neq 0$, Eq. (18) implies that the reflection amplitude is larger if the group velocity dE/dk_x is smaller. This means that if the barrier strength is tuned to produce an almost flat band, even a small impurity potential will lead to a large backscattering.

We find numerically that for a given value of the magnetic field, the strength of the impurity potential which is required to produce a state bound to it is smaller when a potential barrier is present compared to the case when a potential barrier is not present. This is why we set $V_i = \pi$ in Fig. 8 but $V_i = 5\pi$ in Fig. 7. A qualitative reason for this is that a potential barrier already creates

edge states which are localized in one direction (perpendicular to the barrier); then an impurity potential only has to localize such a state in the other direction (along the barrier). Without a potential barrier, the impurity potential by itself has to localize a bound state in two directions.

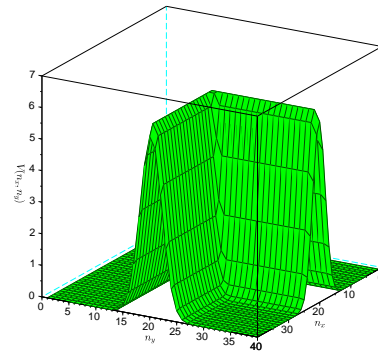


FIG. 9: Surface plot of an “L”-shaped potential. The potential has a width of 2 and a maximum value of $5\pi/(2\sqrt{2}\pi)$ along the spine of the “L”.

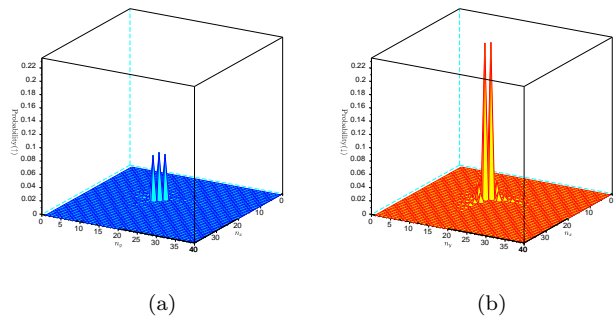


FIG. 10: Surface plots of probabilities of (a) spin- \uparrow and (b) spin- \downarrow for the bound state localized at the corner of an “L”-shaped potential, for $B = \pi/20$ and a system with 40×40 sites.

“L”-shaped potential: Finally, we give an example to show that one can create quasi-one-dimensional systems with bends which can host either localized or extended states of electrons. Fig. 9 shows an “L”-shaped potential barrier consisting of two semi-infinite arms in perpendicular directions; each arm has the form given in Eq. (14) with $\sigma = 2$ and $V_b = 5\pi$. In general we find two kinds of states, one localized at the corner of the “L” and the other running along the arms. An example of a bound state localized at the corner is shown in Fig. 10. Fig. 11 shows an extended wave function which runs along the arms of the potential. (The spin probabilities for this state are in the form of standing waves

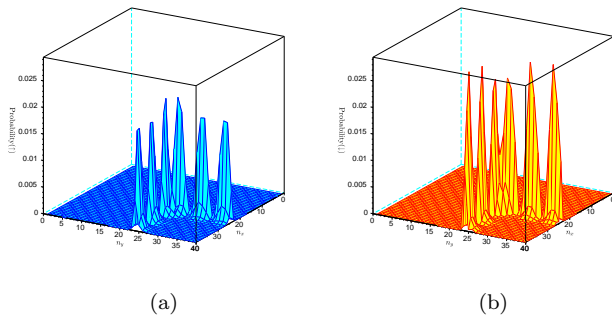


FIG. 11: Surface plots of probabilities of (a) spin- \uparrow and (b) spin- \downarrow for a state which is extended along the arms of an “L”-shaped potential, for $B = \pi/20$ and a system with 40×40 sites.

because of reflections from the edges of the system where we have used open boundary conditions. The wave function would have been a plane wave instead of a standing wave if the system was infinitely large). The ratio of the spin- \downarrow probability to the spin- \uparrow probability is much larger for the state in Fig. 10 compared to the state in Fig. 11. This is because the magnitudes of the momenta k_x and k_y (one or both of which must be complex for a state which is localized in one or both directions) turns out to be much smaller than the magnetic field B for the localized state; hence the wave function is dominated by the magnetic field and therefore has a large component in the direction opposite to it. For the extended state, however, the magnitudes of the momenta turn out to be much larger than B ; hence the wave function is much less affected by the presence of B . Indeed we find numerically that extended states are present if there is only an “L”-shaped potential but no magnetic field, while a bound state can appear at the corner only if a magnetic field is applied.

Physical numbers: We have presented all our numerical results in dimensionless units for convenience. However, we must convert these to some physical numbers in order to think of testing these results experimentally. To do this, let us fix the lattice spacing to be, say, $a = 0.1 \mu\text{m}$. In the absence of a potential and a magnetic field, the dispersion of a massless Dirac electron with momentum k_x is given, on a lattice, by $E = (\hbar v_F/a) \sin(k_x a)$. For the topological insulator Bi_2Se_3 , the velocity on the $x-y$ surface (perpendicular to the quintuple layers) is given by¹¹ $\hbar v_F = 3.33 \text{ eV}\text{\AA}$. This means that the values of energy on the y -axis of Fig. 2 are in units of $\hbar v_F/a = 3.33 \times 10^{-3} \text{ eV}$, and the values of k_x on the x -axis of Figs. 2, 4 and 6 are in units of $1/a = 10 \mu\text{m}^{-1}$. The decay length on the y -axis of Fig. 4 and the x and y coordinates in various figures are all in units of $0.1 \mu\text{m}$. Next, a potential barrier of the form given in Eq. (14) with $V_b = \pi/2$ and $\sigma = 2$ corresponds to a potential whose maximum value is $(V_b/\sigma\sqrt{2\pi})(\hbar v_F/a) = 1.04 \times 10^{-3} \text{ eV}$ and

width is $0.2 \mu\text{m}$. Finally, the Bohr magneton $\mu = e\hbar/(2m_e c) = 5.79 \times 10^{-5} \text{ eV/T}$. Assuming the gyro-magnetic ratio to be $g = 2$ as for a free electron, a value of $B = -g\mu B_z/2 = \pi/20$ corresponds to a magnetic field strength $|B_z| = (\pi/20)(\hbar v_F/a)/(5.79 \times 10^{-5}) = 9.03 \text{ T}$. The numbers given above should only be considered to be rough guidelines; we expect our results for the bound states and their various properties to hold for a range of parameters.

VI. SUMMARY AND DISCUSSION

In this paper, we have used a lattice model to study how a combination of time-reversal invariant (non-magnetic) potentials and a magnetic field can be used to confine Dirac electrons in different geometries. Our main results are as follows.

(i) For an infinitely long potential barrier and no magnetic field, the dispersion of the edge states propagating along the barrier is qualitatively of the form $E = v|k_x|$, where k_x is the momentum along the barrier, if $|k_x|$ is much smaller than the inverse lattice spacing; note that this is quite different from a chiral dispersion which is given by $E = vk_x$. The expectation value of the spin, $\langle \vec{\sigma} \rangle$, of the edge states lies in the y direction. The velocity v of the edge states is smaller than that of the surface states and it can be varied by changing the strength of the potential barrier. The velocity v becomes very small for a particular value of the potential barrier, giving rise to an almost flat band near $E = 0$. The wave function of the edge states decays exponentially away from the potential barrier; the decay length is inversely proportional to $|k_x|$. Hence the edge states will cease to exist when the decay length becomes comparable to the size of the system.

(ii) When a Zeeman field is applied in the z direction, the surface states become gapped but the edge states do not. Further, an edge state now exists even for $k_x = 0$. The spin expectation value develops a component along the z direction. Since the dispersion of the edge states can be controlled by the strength of the potential barrier, the edge states define a tunable one-dimensional system which is separated from the surface states by a gap.

(iii) Next we study what happens when there is a potential localized in some region. In the absence of a Zeeman field such a potential does not produce any localized states. But when a Zeeman field is turned on, we find that exponentially localized states can appear if the potential is strong enough. This gives us a zero-dimensional system.

(iv) We then study a combination of a long potential barrier, a localized potential and a magnetic field; we find that states can appear which are bound to the localized potential. We also study what happens if there is an “L”-shaped potential consisting of two semi-infinitely long arms meeting at a corner and a magnetic field. We find that there can be both states bound to the corner of

the “L” as well as scattering states along the arms.

Our results can be experimentally tested in a number of ways. To begin with, a potential barrier (straight or bent) can be produced by placing an appropriately shaped gate close to the surface of a TI and tuning the gate voltage. Then spin-resolved ARPES can be used to find the energy dispersion and spins of the different edge states. However, this method is not easy to use when a magnetic field is present since the field would affect the trajectories of the electrons emitted from the surface. A second method would be to measure the local density of states using the tunneling conductance from a spin-polarized STM tip which is placed very close to the barrier. If the local density of states is found to be higher when a potential barrier is present compared to the case of no potential, this would provide evidence for the edge states. An almost flat band would give rise to a particularly large density of states at the location of the barrier. Finally, it would be interesting to measure the differential conductance of the quasi-one-dimensional system which is produced by a long potential barrier (either straight or with bends as in an “L”-shaped potential), and study how this varies with the potential barrier or a magnetic field; such a variation would provide indirect evidence for the edge states. Note that since the edge states carry a spin (which is different for opposite edge momenta $+k_x$ and $-k_x$), a non-zero charge conductance along the barrier would also imply a non-zero spin conductance.

We end by pointing out some directions for future work. We have only considered the effects of a Zeeman

coupling to a magnetic field in this work. A magnetic field that has only a Zeeman coupling and no orbital coupling can be realized in a TI by doping with magnetic impurities⁵⁰ or by depositing a ferromagnetic layer on the surface⁵¹. However, one should, in general, study the effects of the orbital coupling of electrons to a magnetic field. In a lattice model, such a coupling can be introduced through the phase in the couplings between nearest neighbor sites following the Peierls prescription.

Our work has shown that in the presence of a magnetic field, one can use potentials of various shapes to form wave guides along which Dirac electrons can propagate. This idea may be used to construct a network of quantum wires by laying down appropriate potentials on the surface of a topological insulator. For this purpose it would be useful to study the scattering matrix and conductance of quasi-one-dimensional systems with “L”-shaped bends and “T”-junctions.

Finally, it would be interesting to study the effect of electron-electron interactions. The almost flat band of states that can be produced by tuning the barrier potential can be a platform for hosting a variety of strongly correlated electron states.

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